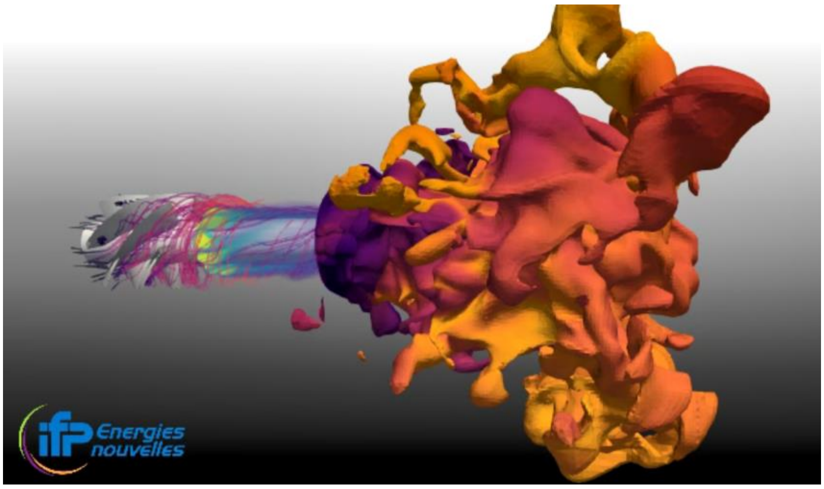
IFP Energies nouvelles is recruiting a postdoctoral researcher:

Set up and exploit 3D CFD simulations for an improved understanding of liquid ammonia injection and combustion in micro-gas turbines

E-fuels obtained from renewable energy stocks are foreseen to play an important role in helping decarbonize the electricity producing and industrial sectors. Among them, ammonia is of high interest as an efficient energy carrier in relation with its capacity as a liquid fuel for a safe and efficient energy storage. It can subsequently be burned in flexible gas turbine powerplants as a single fuel or mixed with hydrogen. In this context, micro gas turbines (MGT) burning ammonia-hydrogen mixtures are a key technology for decentralized energy systems, since they are operationally flexible, and can represent an interesting solution for applications requiring heat at elevated temperatures.

In this context, IFPEN is an active partner of the ADONIS project aiming at producing a technically-sound and accurate assessment of the impact of ammonia and ammonia-hydrogen mixtures on MGT cycle performance for distributed power generation. The collaborative research aims at addressing open questions in terms of fuel injection, combustion dynamics and flame-wall interactions when burning those highly specific fuels, and to deepen the understanding of their impact on the stability, efficiency, pollutant emissions and overall cycle performance of such devices. This is achieved by combining advanced experimental and modelling & simulation approaches performed by two Japanese partners (AIST and Univ. of Tokyo) and five European partners (IFPEN, Silesian Univ. of Technology, SINTEF, Univ. of Orléans and Zürich Univ. of Applied Science), all integrated into the ADONIS consortium funded in the frame of the *CONCERT Japan* program.



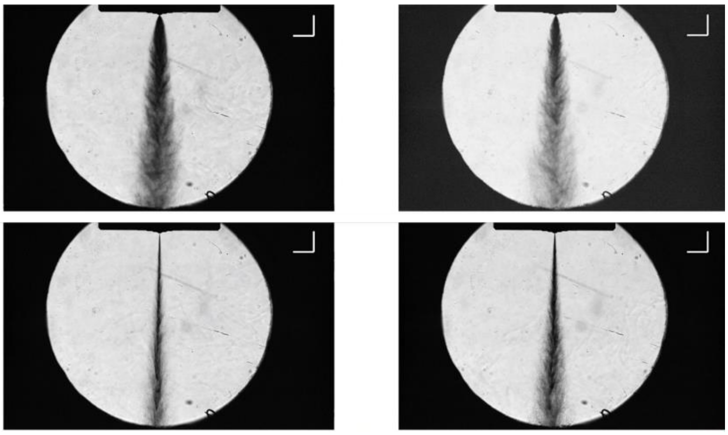
Example of combustion simulation in MGT

Whilst ammonia is usually stored as a liquid, most existing MGT combustors use gaseous ammonia, requiring vaporizers, accumulators and additional heat consumption leading to extra costs and long start up times. Consequently, considering MGT directly fueled with liquid ammonia could allow cost reduction and efficiency improvements. The development of such combustors needs however addressing different challenges. Published studies on gaseous ammonia MGT report a strong influence of mixing in the primary zone of the combustor on flame stabilization and emissions (NOx and unburned NH3). Those difficulties could probably become even more important when burning liquid ammonia. Indeed, its large latent heat of vaporization, as well as the low flame speed of NH3-air mixtures may complexify flame stabilization and promote high unburned fuel emissions. Moreover, the vaporization process needs to be further studied and understood. Thermodynamic conditions encountered in the burner may e.g. lead to flash boiling of the liquid ammonia at the injector exit. Recent experimental studies indicate a very specific behavior of the ammonia spray as a function of the thermodynamic conditions. The high saturation pressure combined with the high latent heat of vaporization induce that a liquid spray can still be observed despite operating under flash boiling conditions, showing that the vaporization process is not instantaneous.

The objective of the 12 months post-doctoral position opening at IFPEN is to set up and perform 3D CFD simulations aimed at contributing to a better understanding of observations reported for different detailed experimental databases on liquid ammonia injection and combustion acquired by the ADONIS partners. The CFD work will be based on the CONVERGE software that includes the required injection and turbulent combustion models, both in terms of RANS and LES approaches, and which will have to be validated and where necessary adapted to ammonia combustion in the course of the post-doc.

The envisaged research work will comprise three main phases:

- The objective of a first phase will be to set up and validate 3D CFD simulations of combustion in the chamber of a MGT fueled with gaseous ammonia, studied experimentally and numerically by other ADONIS partners. By avoiding the difficulties related to liquid injection, the aim will be to concentrate on exploring and modelling aspects related to the turbulent combustion of both pure ammonia and ammonia/hydrogen mixtures. A LES approach using the Thickened Flame Model coupled with an AMR technique developed at IFPEN within CONVERGE will be used to allow a detailed and accurate exploration of the underlying phenomena and of their interactions, and to ease comparisons with experimental findings.
- In parallel, a second phase will be dedicated to set up and validate a 3D CFD model for the liquid injection of ammonia under conditions representative of MGT applications. This will be based on simulations of an experimental database acquired by Univ. of Orléans on liquid ammonia injection into a non-reactive constant volume chamber allowing a detailed characterization of key spray parameters as a function of different injection parameters and operating conditions. By comparing the CFD predictions against experimental findings, the objective will be to yield a better understanding of the underlying physics, and to calibrate the standard spray model to be valid under such very specific conditions.



Example of Amonia spray evolution for different conditions (Univ. of Orléans)

- After having acquired confidence in the spray and combustion modelling, the last phase will aim at simulating a MGT configuration using liquid ammonia injection for which experimental results are available to the ADONIS partners. A coupled simulation of injection and combustion will allow assessing the impact of liquid break-up and vaporization on the mixing and combustion processes for different MGT operating conditions. After having validated the predictions of the developed CFD approach against experimental findings, an extensive and detailed post-processing of the CFD results will aim at contributing to a better mastering of such combustion devices, and to extract first design rules for their future optimization and industrialization. This work will be performed in, close collaboration with the ADONIS project partners.

The successful candidate will be integrated in the applied 3D CFD Team of IFPEN's Mobility & Systems Research Division and will work in close collaboration with IFPEN's CFD model development Department. Moreover, he will exchange and collaborate with the different partners of the ADONIS consortium in charge of experiments and complementary simulation work.

Requested profile and skills:

- PhD in combustion science / multiphase flow modeling
- Experience in 3D CFD modelling and simulations
- Experience with a coding language, ideally Python or C++
- Very good proficiency in written and spoken English; Notions of French not mandatory, yet appreciated

Want to apply ? Send CV and letter of motivation by email to :

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